All data taken at Pacific Northwest National Laboratory (PNNL)
Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov
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Composite spectrum for HCHO_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 1.2362×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Formaldehyde, methylene oxide, methyl aldehyde, methanal, formic aldehyde, oxomethane, formalin, morbicid, veracur, methylene glycol, formalin-40, FYDE, karasan, HCHO, HOCH : [50-00-0]
- Physical properties: fw=30.026 g/mole, fp=–118° C, bp=-19° C
- Supplier and stated purity: Synthesized from paraformaldehyde by heating gently and condensing vapors at liquid nitrogen temperature. Condensate was then cooled to –120 C and pumped on to remove air and CO_2. Sample kept at –50 C to reduce polymerization, minimize polymers and minimize water vapor. Small batches were made as needed to prevent bulk from converting back to paraformaldehyde. Main contaminant was carbon dioxide which has been taken into account and corrected for in composite spectrum. No methanol was observed.
- Sample class: III (PNNL scale). Extremely unstable due to rapid polymerization.
- Temperature of sample: 25.02 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.120, 2.260, 2.4140, 0.2016, 0.7844, 4.13140, 5.13450, 1.57310, 0.2200, 2.07140, 0.51715, 3.4727, 9.535 and 24.86 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -120 C to remove air and CO_2.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 600 cm^{-1} (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm^{-1}
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm^{-1}
- Interferogram zero-fill: 2X
- Apodization: Boxcar
- Phase correction: Mertz
- Beam splitter: Potassium bromide (KBr)
- IR source: Carbide glowbar (22 V)
- Scanner velocity: 60KHz (HeNe crossing frequency)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: 15798 to 0 cm^{-1}

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram (α=0.85, ε=530)

- Composite spectrum created from 14 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.89%, Type B ≤ 10%
- Frequency correction (already applied): V(corrected) = V(instrument)* $0.99999896+8.812x10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide features removed via spectral subtraction. Some residual still observed.
- Baseline correction via 7^{th} order polynomial subtraction